

THE SPECTRUM AND ENERGY LEVELS OF  
DOUBLY IONIZED SCANDIUM (Sc III)

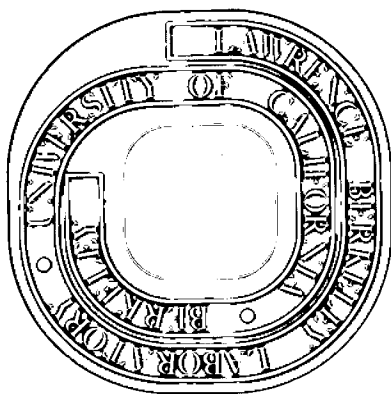
Cor H. H. Van Deurzen, John G. Conway,  
and Sumner P. Davis

August 1972

AEC Contract No. W-7405-eng-48

**For Reference**

**Not to be taken from this room**



## **DISCLAIMER**

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

THE SPECTRUM AND ENERGY LEVELS OF DOUBLY IONIZED SCANDIUM (Sc III)\*

Cor H. H. Van Deurzen

Department of Physics and  
Lawrence Berkeley Laboratory  
University of California  
Berkeley, California 94720

and

John G. Conway

Lawrence Berkeley Laboratory  
University of California  
Berkeley, California 94720

and

Sumner P. Davis

Department of Physics  
University of California  
Berkeley, California 94720

August 1972

ABSTRACT

The spectrum of Sc III has been observed by using a vacuum sliding spark at 250 amp peak current. Excellent separation of the Sc I, II, and III spectra was achieved through careful control over the excitation circuit parameters. In all, 93 lines in the region 550 to 9400 Å are listed which give rise to 24 new levels. The ionization energy of Sc III is revised to  $199677.37 \pm 0.1 \text{ cm}^{-1}$  and series formulae are presented which were used to predict some of the newly found levels to within  $0.25 \text{ cm}^{-1}$ . An isoelectronic comparison of Sc III with KI and Ca II is made.

## INTRODUCTION

The  $\text{Sc}^{2+}$  ion has a ground state  $[\text{Ar}] 3d^1 3^2D_{3/2}$  and is isoelectronic with KI. The analysis of the lower levels by Gibbs and White,<sup>1</sup> as revised by Smith,<sup>2</sup> and the prediction of seven new levels by Russell and Lang<sup>3</sup> (RL) has been confirmed and extended. Several lines observed by others have also been confirmed.<sup>4,5</sup>

It appeared worth renewing investigations of Sc III since there have been developments of ways in which to excite the spectra of lower ionization stages of atoms. The vacuum sliding spark, used in this investigation, operates at low voltage compared with the vacuum spark and affords one some degree of control over which stage of ionization is being excited. Other considerations are the availability of high purity scandium metal rod and high dispersion spectrographic equipment.

# EXPERIMENTAL DETAILS

To excite and separate the spectra of Sc I, II, and III, a vacuum sliding spark was used similar to the one in use at the National Bureau of Standards and the Johns Hopkins University.<sup>6-9</sup> It consists essentially of two  $\frac{1}{4}$ " diameter by 1" cylindrical electrodes of 99.7% pure Sc metal, separated  $\frac{1}{4}$ " by a hollow ( $\frac{1}{8}$ " inside diameter) quartz spacer through which the spark passes. The electrodes are water cooled and the source is operated under a vacuum of about  $5 \times 10^{-6}$  mm of Hg. The LCR electrical circuit is shown in Fig. 1. Separation of the spectra was achieved by varying the circuit parameters L and R which varied the peak current from 10 amp (L and R maximum, Sc I predominates) to 500 amp (L and R minimum, Sc III predominates). Lines belonging to a given stage of ionization were identified by observing their common intensity behaviour with current.

In order to reproduce any setting rather closely, the voltage and current were monitored as shown in Fig. 1. Typical oscillographs of the voltage and current vs. time for two widely separated settings are presented in Fig. 2. At intermediate values of L and R best variation between two consecutive stages of ionization was obtained when the circuit was operated at critical damping,  $R = 2(\frac{L}{C})^{1/2}$ , as indicated on the oscilloscope by a sharp corner at the end of the voltage and current pulses. This control over the circuit was better achieved with the ignitron as a trigger than with the rotating spark gap.

Several different spectrographs were employed to observe the spectra from 500 Å to 9500 Å, a list of which is presented in Table I along with their figures of merit. Calibration spectra below 2680 Å were obtained from a water-cooled copper hollow cathode with Ge and Si in the cathode,<sup>10-12</sup> and above 2680 Å from a ThI electrodeless lamp.<sup>13-15</sup>

## OBSERVATIONS AND DATA REDUCTION

The spectra were first surveyed at 20 Å/mm in air which confirmed the strong Sc III lines predicted by Russell and Lang.<sup>3</sup> More careful separation of the spectra was then obtained at 5 Å/mm in air and 2.78 Å/mm in vacuum. The peak current of 250 amperes, at which the final spectrum was taken, was selected as the minimum excitation where a good number of Sc III lines were present at reasonable exposure times. The Sc III spectrum was then photographed, at a peak current of 250 amperes, from 550 to 2675 Å on the 10.7 m VUV normal-incidence spectrograph at the NBS in Washington; from 2680 to 7900 Å on the  $m\lambda = 225900$  Å grating which obtained the stronger lines (intensity  $\geq 9$ ) in this region; and from 2400 to 9500 Å on the 5 Å/mm grating in order to obtain the remaining weaker lines (at exposures up to  $1\frac{1}{2}$  hrs). Most of the lower wavelength vacuum lines were photographed in the first, second, and third order on the NBS spectrograph. Some of the lines taken on the 5 Å/mm grating were also obtained in multiorders. The weak 9371 Å line could only be obtained on the 20 Å/mm grating.

The lines were in general broad. To avoid possible shifts in the lines due to changing source conditions, much care was taken when photographing the final spectrum to reproduce the same source conditions especially concerning the current and voltage as monitored on the oscilloscope as well as starting with flat electrodes each time a plate was taken. For the 250 amp peak current the circuit parameters were  $V_0 = 800$  volts,  $L = 133$   $\mu$ h,  $C = 24$   $\mu$ f,  $R = 4.5$   $\Omega$ , giving a current-pulse full width at half maximum of 130  $\mu$ sec. The source was fired every 65 msec.

Plate measurements were made on a 25 cm Grant comparator and 25-40 calibration lines used on every 25 cm plate. When fitted with a sixth-order

polynomial the deviation of the calibration lines from their interferometric values was not greater than  $\pm 1.5 \mu \times (\text{dispersion in } \text{\AA}/\text{mm})$ . For some of the wavelengths the fourth decimal was retained as these lines were measured on several plates and all agreed to better than the third decimal, e.g. the 730 and 731  $\text{\AA}$  lines were each measured six times on different plates with an rms deviation of 0.0004  $\text{\AA}$ . The error limits in the wavelengths are thus estimated to be a few units in the last decimal quoted.

Intensities were estimated visually from the plates on a scale 1-350.

## WAVELENGTHS AND ENERGY LEVELS

The list of 93 classified lines is presented in Table II. In the sliding spark spectrum many of the lines were not due to Sc, i.e. oxygen, silicon, and carbon spectra were also present. As a result the weak line at 4642 Å ( $7p^2P_{3/2} - 5d^2D_{5/2}$ ) blends with an OII line and could not be completely resolved at 5 Å/mm. The line at 1742 Å appeared hazy at 2.78 Å/mm and has been identified as the doublet associated with the  $7p-4d$  transition whose fine structure separations differ by  $2.6 \text{ cm}^{-1}$ . This weak line did not show on the NBS plates. The line at 4740.954 was resolved from the Sc I line at 4741.030 on the  $m\lambda = 225900 \text{ Å}$  grating.

Investigation of the structure of Sc III was started on the basis of that given by Smith and the seven levels predicted by RL. There was, however, a  $3 \text{ cm}^{-1}$  discrepancy in the key combination cycle  $3d-4p-4d-4f$  (see Fig. 3) as given by Smith and is due to the 1600 Å and 2000 Å triplets being about 0.06 Å too large. The cycle now closes to within a few hundredths of a wavenumber with the improved wavelengths obtained. Since this discrepancy involved the key vacuum lines  $3d-4p-4d$ , the levels given in Moore's<sup>16</sup> Atomic Energy Levels tables are all too low by about  $2-3 \text{ cm}^{-1}$  with the exception of the 5s which is  $1.3 \text{ cm}^{-1}$  too high due to another discrepancy in the 1895-1912 Å doublet as reported by RL. The 24 newly found levels and the corrected values for the previously known levels are presented in Table III.

In Table III is also displayed the usual near-constancy of the difference  $\Delta n^*$  for the two components of a doublet level in a Rydberg series, which was used to predict the fine structure interval of the next level above the last observed one. In closing the combination cycles, agreement was



found to within a few units in the second decimal place, i.e. within the experimental error, indicating that it was possible to maintain sufficient control over excitation to achieve internal consistency.

## IONIZATION ENERGY AND SERIES FORMULAE

The ionization energy of an atom can be calculated from a series which is assumed to obey a Ritz-like formula and in essence extrapolating the series to the limit  $n = \infty$ .<sup>17</sup> The  $ng$  series which reaches closest to the limit and most nearly obeys the simple two-parameter Ritz formula is assumed to give the best value for the ionization energy. A calculation based on the four observed members (5-8) of the  $ng$  series in Sc III results in

$$\delta_n \equiv n - n^* = 9.153908 \times 10^{-2} - 7.04772 \times 10^{-8} T_n - 1.9855 \times 10^{-14} T_n^2$$

$$E_{\text{ion}} = 199677.37 \text{ cm}^{-1}$$

where  $T_n \equiv R \left( \frac{Z_c}{n^*} \right)^2$  is the  $n^{\text{th}}$  term in the series.

Similar calculations carried out on the four highest observed members of the other series give the ionization energies presented in column three of Table IV. For further comparison and to indicate how nearly the  $ng$  series obeys the simple Ritz formula, the results using only a) the first three and b) the last three observed members of this series are also presented. They agree with the above value to within  $0.08 \text{ cm}^{-1}$ . The rather large difference between the value obtained from the  $nd$  series and the values derived from the other series is most likely due to the quadratic formula for  $\delta_n$  being inadequate to represent the core effects on the  $nd$  series. (The calculation based on the 3d-6d terms results in  $199807 \text{ cm}^{-1}$  whereas the 4d-7d gives  $199683 \text{ cm}^{-1}$ .) Until more levels are found, we adopt

$$E_{\text{ion}} = 199677.37 \pm 0.1 \text{ cm}^{-1} .$$

With the ionization energy derived, it was possible to attempt to represent unperturbed series by formulae and thus predict the next level in the series. This was done using an extended Ritz formula for the quantum defect

$$\delta_n \equiv n - n^* = a + bt_n + ct_n^2 + dt_n^3 + et_n^4$$

$$t_n \equiv \frac{T_n}{RZ_c^2} = \left(\frac{1}{n^*}\right)^2$$

where  $T_n$  is the  $n^{\text{th}}$  term,  $R$  is the mass-corrected Rydberg constant<sup>†</sup> and  $Z_c$  is the net core charge, set to three for Sc III.<sup>17,18</sup> This procedure allowed the choice of one more constant than the method used in the foregoing to obtain three constants and the correction to the trial ionization energy. In the computer program set up, at least one of the last four constants had to be set to zero. In Table IV are listed the appropriate constants obtained from the indicated members of the series using the ionization energy  $199677.37 \text{ cm}^{-1}$ . For the nd series the fit to the experimental data was improved when the constant d was set to zero instead of e (3d-6d with the constants abcd predicted the observed  $7d^2D_{3/2}$  level  $1.4 \text{ cm}^{-1}$  too high whereas with the abce constants it was  $0.25 \text{ cm}^{-1}$  too high). The listed constants were then used to predict the next term above the last observed one using an iterative procedure on the predicted value of  $T$  until  $|T(I+1) - T(I)| \leq 10^{-3} \text{ cm}^{-1}$ , usually satisfied in one or two steps. In column 9 are given the values of  $T_{\text{obs}} - T_{\text{calc}}$  for the last observed term using all of the lower levels with their respective

<sup>†</sup>For scandium  $R = (109737.31 - \frac{60.22}{44.956}) \text{ cm}^{-1}$  was used.

constants. In this manner the weak lines concerning the 7p and 7d levels were found, and the levels derived from them agreed with the predicted values to within  $0.25 \text{ cm}^{-1}$ . Applying the theory of atom-core polarization for "non-penetrating" orbits<sup>19,20</sup> to calculate the departure from hydrogenic term values, we obtained from the ng series the value  $\alpha = 0.34 \times 10^{-24} \text{ cm}^3$  for the polarizability of the ion  $\text{Sc}^{2+}$ . With this value the 6h-8h terms were predicted to be  $T_{6h} = 27455 \text{ cm}^{-1}$ ,  $T_{7h} = 20170 \text{ cm}^{-1}$ , and  $T_{8h} = 15442 \text{ cm}^{-1}$ . The lines involving all the given predicted levels were looked for but not found, presumably because of their low intensity.

# ISOELECTRONIC SEQUENCE

With the first two spectra of the KI isoelectronic sequence well analyzed it was possible to observe how the Sc III energy levels fit into the sequence. Figure 4 shows that the 4f and 5g levels of Sc III complete a smooth curve from KI to Ti IV and V V. The trends, shown for the highest observed levels in Sc III, show a smooth curve and have now been established with improved accuracy. It is in Sc III that the 7d level first lies below the 8s level.

### CONCLUSION

This research has confirmed and extended the knowledge of the doubly ionized state of Sc. The study of the spectra produced by the vacuum sliding spark provides additional information on spectra separation of lower ionization stages of atoms. Internal consistency was obtained in the level system derived from the spectrum at constant source conditions. It would be of interest to study the line and level variation with varying source conditions.

ACKNOWLEDGEMENTS

The authors wish to thank Dr. W. C. Martin and the spectroscopy group at the National Bureau of Standards in Washington for making their high resolution spectrograph available, and especially Dr. V. Kaufman for generously giving of his time while taking the spectra there. Also George V. Shalimoff of LBL for his help.

# FOOTNOTES AND REFERENCES

\* Work performed under the auspices of the U. S. Atomic Energy Commission and a grant from the National Science Foundation. A preliminary report of this work was given at the 1972 Spring meeting of the Optical Society of America [J. Opt. Soc. Am. 62, 714 (1972)].

1. R. C. Gibbs and H. E. White, Proc. Nat. Acad. Sci. 12, 599 (1926).
2. Stanley Smith, Proc. Nat. Acad. Sci. 13, 66 (1927).
3. H. N. Russell and R. J. Lang, Astroph. J. 66, 19 (1927).
4. A. Beckman, Bidrag till kännedomen om skandiums specktrum i yttersta ultraviolett (Almqvist and Wiksell, Uppsala, 1937).
5. R. Buchta, L. J. Curtis, I. Martinson, and J. Brzozowski, Physica Scripta 4, 55 (1971).
6. G. H. Dieke, H. M. Crosswhite, and B. Dunn, J. Opt. Soc. Am. 51, 820 (1961).
7. Wm. R. Callahan, J. Opt. Soc. Am. 53, 695 (1963).
8. Jack Sugar, J. Opt. Soc. Am. 53, 831 (1963).
9. Joseph Reader, Gabriel L. Epstein, and Jan Olof Ekberg, J. Opt. Soc. Am. 62, 273 (1972).
10. V. Kaufman, L. J. Radziemski, Jr., and K. L. Andrew, J. Opt. Soc. Am. 56, 911 (1966).
11. L. J. Radziemski, Jr., K. L. Andrew, V. Kaufman, and U. Litzén, J. Opt. Soc. Am. 57, 336 (1967).
12. V. Kaufman and J. F. Ward, J. Opt. Soc. Am. 56, 1591 (1966).
13. Francisco P. J. Valero, J. Opt. Soc. Am. 58, 484 (1968).
14. David Goorvitch, Francisco P. J. Valero, and Alicia L. Clúa, J. Opt. Soc. Am. 59, 971 (1969).



15. A. Giacchetti, R. W. Stanley, and R. Zalubas, J. Opt. Soc. Am. 60, 474 (1970).
16. C. E. Moore, Atomic Energy Levels, Vol. I, Natl. Bur. Std. (U.S.) circ. No. 467 (U. S. Government Printing Office, Washington, D. C., 1949).
17. A. G. Shenstone, Phil. Trans. Roy. Soc. London A235, 195 (1936).
18. Bengt Edlén and Percy Risberg, Ark. Fys. 10, 553 (1956).
19. M. Born and W. Heisenberg, Z. Phys. 23, 388 (1924).
20. I. Waller, Z. Phys. 38, 635 (1926).

Table I. Spectrographs used to record the spectra of Sc I, II, and III.

Focal length (m)	Grooves/mm	$m\lambda$ (at blaze) (order $\times$ Å)	$m \frac{d\lambda}{dx}$ (order $\times$ Å/mm)	
3.4 (Jarrell-Ash)	79	225900	17.5	air
3.4 ( " )	600	5000	5.2	"
0.75 ( " )	600	7000	20	"
10.7 ( " ) (NBS)	1200	1200	0.78	vacuum
3 (McPherson)	1200	1380	2.78	"

Table II. Lines of Sc III

Level combination	Wave number ( $\text{cm}^{-1}$ )	Wavelength ( $\text{\AA}$ )	Intensity
$6p^2P_{1/2} - 7s^2S_{1/2}$	10667.45	9371.74	1
$4f^2F_{5/2} - 5d^2D_{3/2}$	11256.16	8881.585	15
$4f^2F_{7/2} - 5d^2D_{5/2}$	11276.08	8865.891	30
$5d^2D_{5/2} - 5f^2F_{7/2}$	11322.19	8829.785	50
$5d^2D_{3/2} - 5f^2F_{5/2}$	11342.12	8814.276	35
$5g^2G - 6f^2F$	11715.46	8533.383	2
$6f^2F - 8g^2G$	12426.97	8044.799	1
$5f^2F - 6g^2G$	12705.17	7868.648	70
$5s^2S_{1/2} - 5p^2P_{1/2}$	13244.64	7548.148	70
$5s^2S_{1/2} - 5p^2P_{3/2}$	13420.65	7449.155	90
$6d^2D_{5/2} - 7f^2F_{7/2}$	13611.43	7344.746	1
$6d^2D_{3/2} - 7f^2F_{5/2}$	13622.02	7339.033	1
$4d^2D_{3/2} - 5p^2P_{1/2}$	15849.52	6307.595	60
$4d^2D_{5/2} - 5p^2P_{3/2}$	15980.21	6256.010	80
$5f^2F_{5/2} - 7d^2D_{3/2}$	15984.67	6254.264	1
$5f^2F_{7/2} - 7d^2D_{5/2}$	15991.23	6251.698	1
$4d^2D_{3/2} - 5p^2P_{3/2}$	16025.54	6238.314	10
$5p^2P_{3/2} - 5d^2D_{3/2}$	19846.86	5037.176	9
$5p^2P_{3/2} - 5d^2D_{5/2}$	19866.93	5032.087	60
$6p^2P_{3/2} - 7d^2D_{5/2}$	19888.36	5026.665	2
$6p^2P_{1/2} - 7d^2D_{3/2}$	19967.25	5006.804	1
$5f^2F - 7g^2G$	20004.97	4997.365	6

(continued)

Table II (continued)

Level combination	Wave number ( $\text{cm}^{-1}$ )	Wavelength ( $\text{\AA}$ )	Intensity
$5p^2P_{1/2} - 5d^2D_{3/2}$	20022.91	4992.886	50
$6p^2P_{3/2} - 8s^2S_{1/2}$	20220.60	4944.072	1
$5p^2P_{3/2} - 6s^2S_{1/2}$	20910.86	4780.868	15
$5p^2P_{1/2} - 6s^2S_{1/2}$	21086.90	4740.954	10
$7p^2P_{1/2} - 5d^2D_{3/2}$	21507.93	4648.148	1
$7p^2P_{3/2} - 5d^2D_{5/2}$	21536.0	4642.08	2b
$4f^2F - 5g^2G$	23198.18	4309.471	40
$5d^2D_{5/2} - 6f^2F_{7/2}$	23637.52	4229.371	6
$5d^2D_{3/2} - 6f^2F_{5/2}$	23657.61	4225.779	6
$4d^2D_{5/2} - 4f^2F_{7/2}$	24571.17	4068.661	100
$4d^2D_{3/2} - 4f^2F_{5/2}$	24616.25	4061.209	80
$5f^2F - 8g^2G$	24742.36	4040.510	6
$4f^2F_{5/2} - 6d^2D_{3/2}$	28718.63	3481.064	5
$4f^2F_{7/2} - 6d^2D_{5/2}$	28729.19	3479.785	6
$4f^2F - 6g^2G$	35303.42	2831.754	10
$4s^2S_{1/2} - 4p^2P_{1/2}$	36564.98	2734.048	230
$4s^2S_{1/2} - 4p^2P_{3/2}$	37038.85	2699.067	350
$5p^2P_{3/2} - 6d^2D_{3/2}$	37309.41	2679.493	1
$5p^2P_{3/2} - 6d^2D_{5/2}$	37320.10	2678.725	8
$5p^2P_{1/2} - 6d^2D_{3/2}$	37485.47	2666.907	6
$5p^2P_{3/2} - 7s^2S_{1/2}$	37874.02	2639.546	2
$5p^2P_{1/2} - 7s^2S_{1/2}$	38050.05	2627.334	1

(continued)

Table II (continued)

Level combination	Wave number ( $\text{cm}^{-1}$ )	Wavelength ( $\text{\AA}$ )	Intensity
$5s^2S_{1/2} - 6p^2P_{3/2}$	40712.3	2455.52	1
$4f^2F - 7g^2G$	42603.27	2347.238*	6
$4d^2D_{3/2} - 6p^2P_{1/2}$	43232.16	2313.093*	6
$4d^2D_{5/2} - 6p^2P_{3/2}$	43272.25	2310.950*	7
$4d^2D_{3/2} - 6p^2P_{3/2}$	43317.58	2308.532*	5
$5p^2P_{3/2} - 7d^2D_{3/2}$	47173.64	2119.828*	1
$5p^2P_{3/2} - 7d^2D_{5/2}$	47180.41	2119.524*	5
$4f^2F - 8g^2G$	47340.62	2112.351*	1
$5p^2P_{1/2} - 7d^2D_{3/2}$	47349.89	2111.937*	2
$5p^2P_{3/2} - 8s^2S_{1/2}$	47512.51	2104.709*	2
$5p^2P_{1/2} - 8s^2S_{1/2}$	47688.6	2096.94 *	1
$4p^2P_{3/2} - 4d^2D_{3/2}$	49679.42	2012.906*	50
$4p^2P_{3/2} - 4d^2D_{5/2}$	49724.77	2011.070*	160
$4p^2P_{1/2} - 4d^2D_{3/2}$	50153.31	1993.886	90
$4p^2P_{3/2} - 5s^2S_{1/2}$	52284.29	1912.620	60
$4p^2P_{1/2} - 5s^2S_{1/2}$	52758.18	1895.441	40
$7p^2P - 4d^2D$	57382.7	1742.69	2h
$4d^2D_{5/2} - 6f^2F_{7/2}$	59484.69	1681.105	7
$4d^2D_{3/2} - 6f^2F_{5/2}$	59530.03	1679.824	5
$3d^2D_{3/2} - 4p^2P_{1/2}$	62104.30	1610.1945	150
$3d^2D_{5/2} - 4p^2P_{3/2}$	62380.55	1603.0637	180
$3d^2D_{3/2} - 4p^2P_{3/2}$	62578.16	1598.002	80

(continued)

Table II (continued)

Level combination	Wave number ( $\text{cm}^{-1}$ )	Wavelength ( $\text{\AA}$ )	Intensity
$4d^2D_{5/2} - 7f^2F_{7/2}$	66911.73	1494.506	1
$4d^2D_{3/2} - 7f^2F_{5/2}$	66956.75	1493.502	1
$4p^2P_{3/2} - 5d^2D_{3/2}$	85551.78	1168.883	10
$4p^2P_{3/2} - 5d^2D_{5/2}$	85571.92	1168.6077	25
$4p^2P_{1/2} - 5d^2D_{3/2}$	86025.72	1162.4431	20
$4p^2P_{3/2} - 6s^2S_{1/2}$	86615.87	1154.523	20
$4p^2P_{1/2} - 6s^2S_{1/2}$	87089.75	1148.241	15
$4s^2S_{1/2} - 5p^2P_{1/2}$	102567.8	974.965	6
$4s^2S_{1/2} - 5p^2P_{3/2}$	102743.8	973.295	8
$4p^2P_{3/2} - 6d^2D_{5/2}$	103025.1	970.638	4
$4p^2P_{1/2} - 6d^2D_{3/2}$	103488.3	966.293	3
$4p^2P_{3/2} - 7s^2S_{1/2}$	103578.81	965.4484	4
$4p^2P_{1/2} - 7s^2S_{1/2}$	104052.7	961.052	2
$3d^2D_{5/2} - 5p^2P_{3/2}$	128085.5	780.729	8
$3d^2D_{3/2} - 5p^2P_{1/2}$	128107.14	780.5966	6
$4s^2S_{1/2} - 6p^2P_{1/2}$	129950.4	769.524	1
$4s^2S_{1/2} - 6p^2P_{3/2}$	130035.9	769.019	1
$3d^2D_{5/2} - 4f^2F_{7/2}$	136676.45	731.6549	15
$3d^2D_{3/2} - 4f^2F_{5/2}$	136873.86	730.5997	10
$3d^2D_{5/2} - 6p^2P_{3/2}$	155376.7	643.597	2
$3d^2D_{3/2} - 6p^2P_{1/2}$	155488.8	643.133	2
$3d^2D_{5/2} - 5f^2F_{7/2}$	159274.60	627.8465	8

(continued)

Table II (continued)

Level combination	Wave number ( $\text{cm}^{-1}$ )	Wavelength ( $\text{\AA}$ )	Intensity
$3d^2D_{3/2} - 5f^2F_{5/2}$	159472.00	627.0693	7
$3d^2D_{5/2} - 6f^2F_{7/2}$	171589.99	582.7846	3
$3d^2D_{3/2} - 6f^2F_{5/2}$	171787.52	582.1144	2
$3d^2D_{5/2} - 7f^2F_{7/2}$	179016.6	558.608	1
$3d^2D_{3/2} - 7f^2F_{5/2}$	179213.2	557.995	1

b - Blends with an OII line.

h - Hazy.

\* - Wavelength in vacuum as measured.

Table III. Energy levels of Sc III.

Symbol	Energy ( $\text{cm}^{-1}$ )	Interval ( $\text{cm}^{-1}$ )	Term Value ( $\text{cm}^{-1}$ )	$n^*$	$\Delta n^*$
$4s^2S_{1/2}$	25539.32		174138.05	2.381491	
$5s^2S_{1/2}$	114862.48		84814.89	3.412398	
$6s^2S_{1/2}$	149194.03		50483.34	4.423049	
$7s^2S_{1/2}$	166157.17		33520.20	5.428033	
$8s^2S_{1/2}$	175795.73		23881.64	6.430781	
$9s^2S_{1/2}$	(181799) <sup>a</sup>		(17878)		
$4p^2P_{1/2}$	62104.30	473.88	137573.07	2.679348	0.004626
$^2P_{3/2}$	62578.18		137099.19	2.683974	
$5p^2P_{1/2}$	128107.12	176.03	71570.25	3.714749	0.004577
$^2P_{3/2}$	128283.15		71394.22	3.719326	
$6p^2P_{1/2}$	155489.78	85.42	44187.59	4.727653	0.004576
$^2P_{3/2}$	155575.20		44102.17	4.732229	
$7p^2P_{1/2}$	169637.96	47.9	30039.41	5.733899	0.00458
$^2P_{3/2}$	169685.9		29991.5	5.73848	
$8p^2P_{1/2}$	(177920)	(29.6)	(21757)		
$^2P_{3/2}$	(177950)		(21728)		
$3d^2D_{3/2}$	0.00	197.64	199677.37	2.223982	0.001102
$^2D_{5/2}$	197.64		199479.73	2.225084	
$4d^2D_{3/2}$	112257.62	45.33	87419.75	3.361174	0.000872
$^2D_{5/2}$	112302.95		87374.42	3.362046	

<sup>a</sup>Predicted levels.

(contd.)



Table III. (continued)

Symbol	Energy (cm <sup>-1</sup> )	Interval (cm <sup>-1</sup> )	Term Value (cm <sup>-1</sup> )	n*	Δn*
5d <sup>2</sup> D <sub>3/2</sub>	148130.03	20.11	51547.34	4.377162	0.000854
2D <sub>5/2</sub>	148150.14		51527.23	4.378016	
6d <sup>2</sup> D <sub>3/2</sub>	165592.55	10.74	34084.82	5.382887	0.000848
2D <sub>5/2</sub>	165603.29		34074.08	5.383735	
7d <sup>2</sup> D <sub>3/2</sub>	175457.03	6.53	24220.34	6.385658	0.000860
2D <sub>5/2</sub>	175463.56		24213.81	6.386518	
8d <sup>2</sup> D <sub>3/2</sub>	(181579)	(4.3)	(18098)		
2D <sub>5/2</sub>	(181584)		(18094)		
4f <sup>2</sup> F <sub>5/2</sub>	136873.87	.25	62803.50	3.965554	0.000008
2F <sub>7/2</sub>	136874.12		62803.25	3.965562	
5f <sup>2</sup> F	159472.24		40205.13	4.956271	
6f <sup>2</sup> F	171787.64		27889.73	5.950776	
7f <sup>2</sup> F	179214.70		20462.67	6.947277	
8f <sup>2</sup> F	(184031)		(15646)		
5g <sup>2</sup> G	160072.18		39605.19	4.993668	
6g <sup>2</sup> G	172177.41		27499.96	5.992799	
7g <sup>2</sup> G	179477.24		20200.13	6.992278	
8g <sup>2</sup> G	184214.61		15462.76	7.991941	
9g <sup>2</sup> G	(187462)		(12215)		

Table IV. Ionization energies of the different series, and constants for the series formulae used for predictions.

Series Members	J	Ionization Energy ( $\text{cm}^{-1}$ )	Formula Constants				$T_{\text{obs}} - T_{\text{calc}}$ ( $\text{cm}^{-1}$ )	$T_{\text{predicted}}$ ( $\text{cm}^{-1}$ )
			a	b	c	d		
5s-8s	1/2	199677.28	1.562680	0.26241	0.3354	-0.137	0	17878.3
4p-7p	1/2	199676.88	1.253807	0.38231	0.7245	-0.173	0	21757.3
	3/2	199676.91	1.249202	0.38372	0.7263	-0.164	0	21727.7
4d-7d	3/2	199682.69	0.608772	0.19325	1.3584	0	+37.55	18097.9
	5/2	199683.30	0.607810	0.19965	1.2661	0	+41.98	18093.6
4f-7f	7/2	199676.15	0.063190	-0.53737	1.6555	-4.958	0	15646.3
5g-8g	7/2, 9/2	199677.37	0.0091529	-0.06949	-0.0234	0.046	0	12215.4
5g-7g	7/2, 9/2	199677.45*	0.0091539	-0.06960	-0.0194	0	0	12215.4
6g-8g	7/2, 9/2	199677.40*	0.0091533	-0.06955	-0.0205	0	0	12215.4

\* Calculated using the simple two-parameter Ritz formula

FIGURE CAPTIONS

Fig. 1. Schematic of the electrical circuit used to excite and separate the spectra of Sc I, II, and III. To trigger the circuit either a rotating spark gap or an ignitron was used.

Fig. 2. Voltage across and current through the light source.

Top:  $L = 68 \mu\text{h}$ ,  $C = 24 \mu\text{f}$ ,  $R = 2(L/C)^{1/2}$  (critically damped).

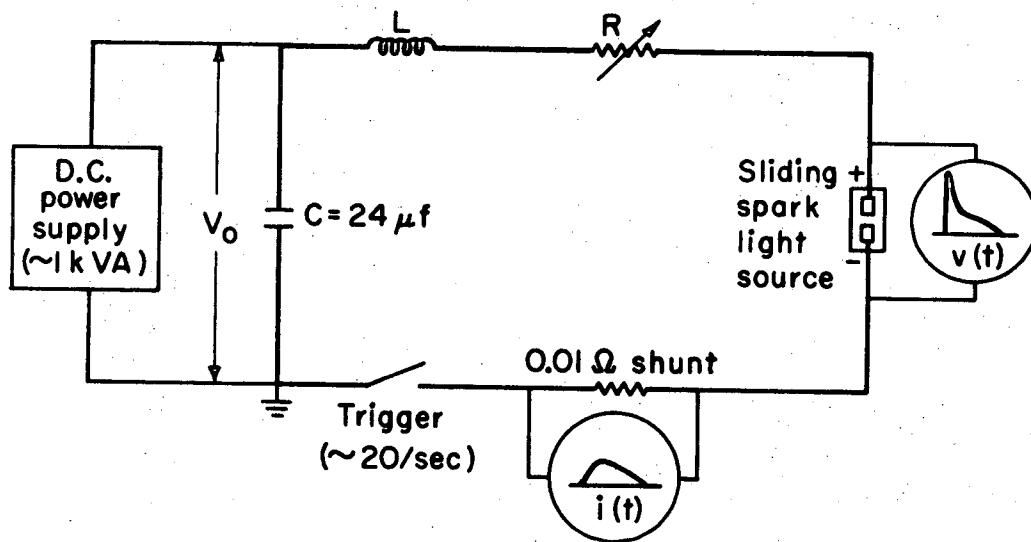
Excites mainly Sc III and spacer impurities.

Bottom:  $L = 860 \mu\text{h}$ ,  $C = 24 \mu\text{f}$ ,  $R = 14 \Omega$  (slightly overdamped).

Excites mainly Sc I, and II, and only the strongest lines of Sc III.

Fig. 3. Energy level diagram for Sc III. The figures give the approximate wavelength of the leading line in each multiplet. The dotted lines are the next predicted levels.

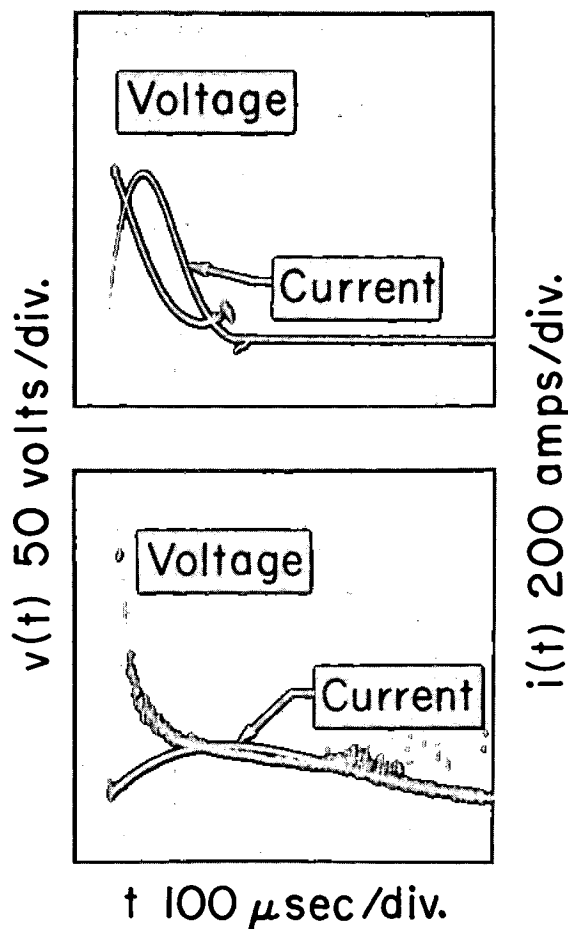
Fig. 4. Isoelectronic sequence for selected levels.



Voltage  $600 \leq V_0 \leq 900$  volts  
 Inductance  $15 \leq L \leq 1100 \mu h$   
 Resistance  $1 \leq R \leq 150 \Omega$

Fig. 1. Schematic of the electrical circuit used to excite and separate the spectra of Sc I, II, and III. To trigger the circuit either a rotating spark gap or an ignitron was used.

XBL728-3757



XBB 428-4122

Fig. 2. Voltage across and current through the light source.

Top:  $L = 68 \mu\text{h}$ ,  $C = 24 \mu\text{f}$ ,  $R = 2(L/C)^{1/2}$  (critically damped).

Excites mainly Sc III and spacer impurities.

Bottom:  $L = 860 \mu\text{h}$ ,  $C = 24 \mu\text{f}$ ,  $R = 14 \Omega$  (slightly overdamped).

Excites mainly Sc I, and II, and only the strongest lines of Sc III.

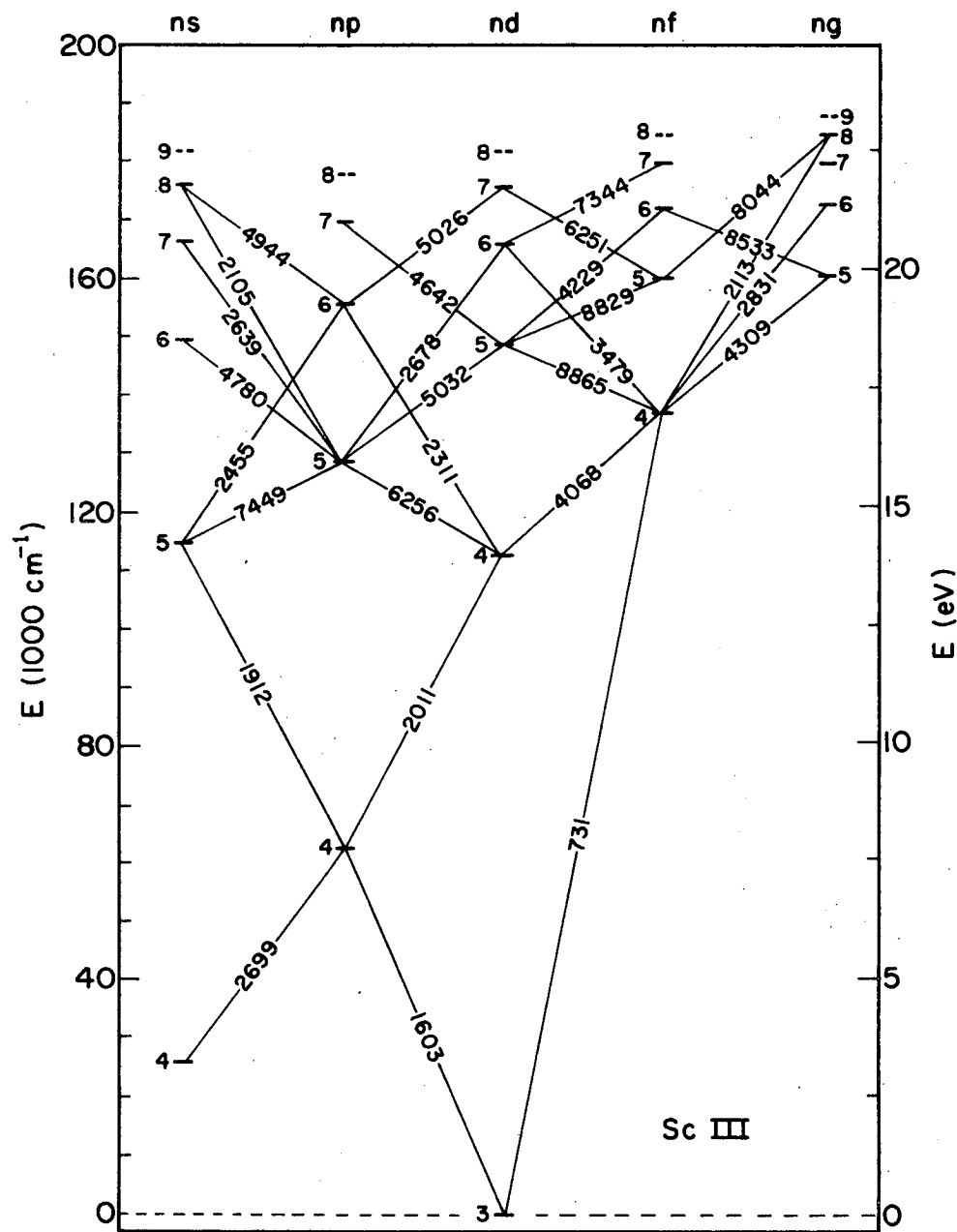


Fig. 3. Energy level diagram for Sc III. The figures give the approximate wavelength of the leading line in each multiplet. The dotted lines are the next predicted levels.

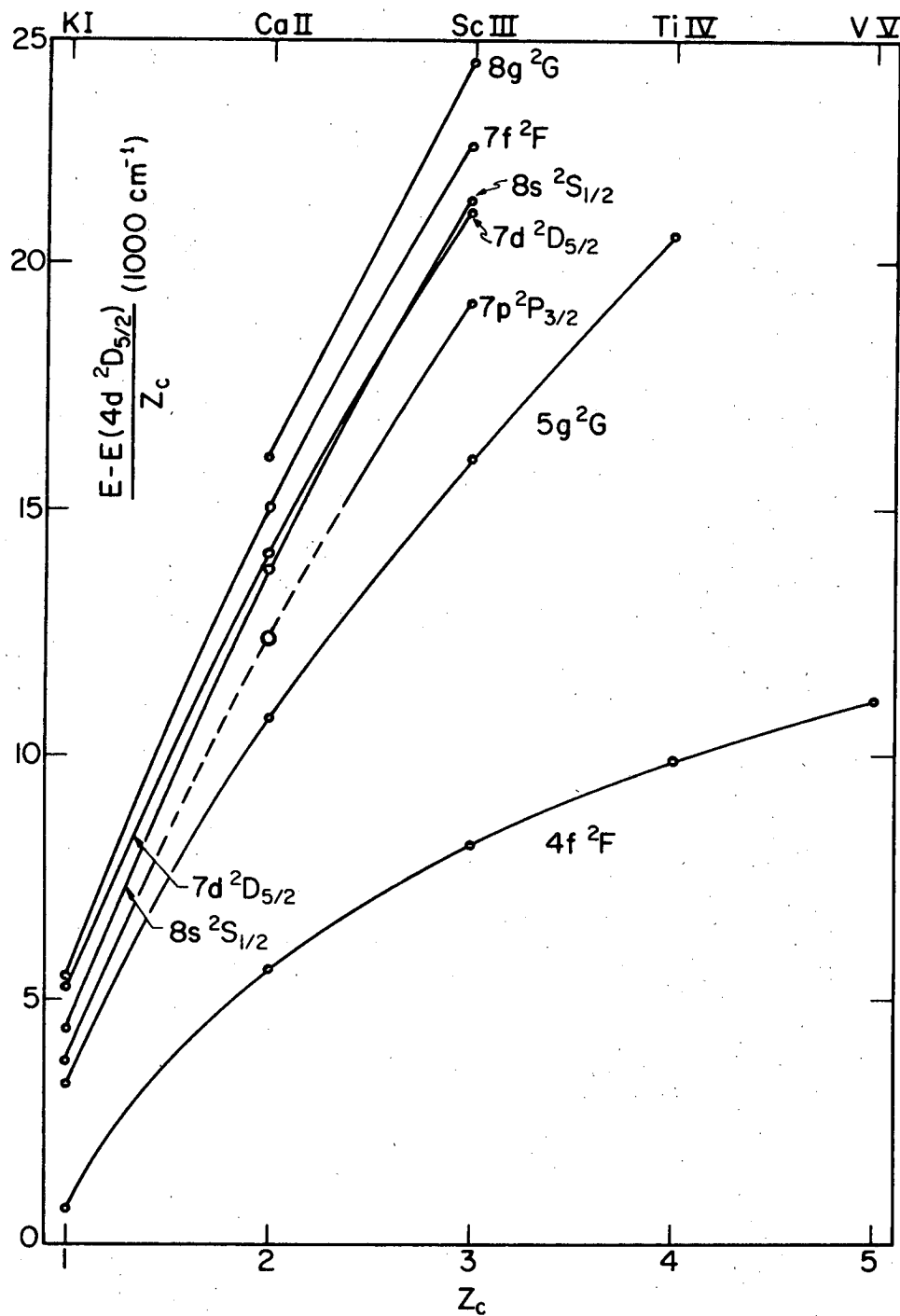


Fig. 4. Isoelectronic sequence for selected levels.

XBL728-3758

#### LEGAL NOTICE

*This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Atomic Energy Commission, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.*



TECHNICAL INFORMATION DIVISION  
LAWRENCE BERKELEY LABORATORY  
UNIVERSITY OF CALIFORNIA  
BERKELEY, CALIFORNIA 94720